2014-01-2718
Published 10/13/2014

doi:10.4271/2014-01-2718
saefuel.saejournals.org

Octane Appetite: The Relevance of a Lower Limit to the MON Specification in a Downsized, Highly Boosted DISI Engine

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ABSTRACT

Market demand for high performance gasoline vehicles and increasingly strict government emissions regulations are driving the development of highly downsized, boosted direct injection engines. The in-cylinder temperatures and pressures of these emerging technologies tend to no longer adhere to the test conditions defining the RON and MON octane rating scales. This divergence between fuel knock rating methods and fuel performance in modern engines has previously led to the development of an engine and operating condition dependent scaling factor, K, which allows for extrapolation of RON and MON values. Downsized, boosted DISI engines have been generally shown to have negative K-values when knock limited, indicating a preference for fuels of higher sensitivity and challenging the relevance of a lower limit to the MON specification.

The Ultraboost engine is an inline-4 downsized, highly boosted prototype DISI engine designed to achieve a 35% reduction in CO_2 emissions whilst maintaining performance of a production V8. A series of 14 fuel formulations were tested to probe engine response to various fuel properties. This paper presents results from a 7 fuel RON and MON decorrelated matrix at four high-load engine conditions. The K-value was found to be negative at all engine conditions; fuels of higher sensitivity were found to yield improved engine performance. Furthermore, in-cylinder experimental data from high load knocking conditions with a single standard octane fuel were used to simulate the K-value; a similar trend between theory and experiment was observed.

CITATION: Remmert, S., Campbell, S., Cracknell, R., Schuetze, A. et al., "Octane Appetite: The Relevance of a Lower Limit to the MON Specification in a Downsized, Highly Boosted DISI Engine," *SAE Int. J. Fuels Lubr.* 7(3):2014, doi:10.4271/2014-01-2718.

INTRODUCTION

Octane Appetite

Modern spark-ignition engine development is driven by the balance between meeting emissions legislation and maintaining vehicle performance to meet consumer demand. For a given engine configuration and operating condition, efficiency and performance can best be achieved via a sufficiently advanced spark timing (Minimum (advance) for Best Torque, MBT) that allows for optimal combustion phasing. Fuel formulation can have a direct impact on an engine's ability to achieve MBT and hence optimal performance, as the spark advance can be restricted by potentially damaging auto-ignition of the end-gas ahead of the flame front, known as knock [1].

A fuel's knock resistance is historically characterised by the research octane number (RON) and motor octane number (MON) determined in a Cooperative Fuels Research (CFR) engine [2]. RON and MON are assigned by determining the volume percent of iso-octane in a binary mixture with n-heptane -the resulting mixture known as a primary reference fuel (PRF) - required to reproduce the knocking behaviour of a

real fuel. The MON test uses a higher temperature, lower manifold pressure and higher engine speed condition than RON, as shown in Table 1.

Table 1. CFR Engine Conditions for RON and MON Tests

Property	RON Test	MON Test
ASTM Method	D-2699	D-2700
Engine Speed (rpm)	600	900
Intake Temperature (˚C)	52	149
Spark Advance (CAD aTDC)	-13	-19 to -26

Due to specific equilibrium chemistry resulting in non-Arrhenius reaction rate for the ignition delay behaviour between 650-900 K, paraffinic fuels exhibit increased knock-resistance under MON conditions and therefore have low sensitivity, defined as *S = RON - MON* [2, 3]. Real fuels - which also contain olefins and aromatics - do not exhibit negative temperature coefficient (NTC) behaviour and thus have higher fuel sensitivity. This phenomenon highlights two problems with the industry standard octane rating method: (1) the rating scale is defined by paraffins, which do not represent the auto-ignition behaviour of a real fuel, and (2) the knock propensity of a real, sensitive fuel depends on the in-cylinder temperature and pressure history which can change with engine design and operating condition.

Modern engines tend towards downsized, direct injection technologies, with increased charging, and employ the highest compression ratios consistent with this charging. Direct injection, more efficient breathing and improved inlet system, head and block design to reduce charge heating, all result in higher pressures and lower temperatures in-cylinder for modern engines relative to the traditional RON and MON tests [4]. Furthermore, inter-cooling and the introduction of cooled external EGR to the cylinder will decrease the temperature for a given pressure even further [5]. Due to the apparent disconnect between modern engine conditions and the CFR engine - on which the octane rating scales are defined - a series of recent studies have called into question the relevance of the RON and especially MON specifications in predicting fuel knocking propensity [1, 3, 4, 6, 7, 8, 9].

To extrapolate RON and MON test results to relevant engine conditions, it is useful to define the octane index (OI) as a linear combination of RON and MON with an engine condition dependent weighting factor, K [1]:

$$OI = RON - K \times (RON - MON) = RON - K \times S \quad (1)$$

The K-value is thought to be dependent only on the in-cylinder temperature and pressure history experienced by the end-gas prior to the onset of auto-ignition. OI defines a PRF composition with the same auto-ignition behaviour as a real fuel *at a given engine operating condition*; the higher the OI of a given fuel, the more resistant it is to knock [7].

As can be seen in equation (1), the OI is equivalent to RON or MON when K=0 or K=1, respectively. K is traditionally assumed to be positive; indeed, the anti-knock index (AKI) of the US market is equivalent to OI when K=0.5. However, studies in research engines [1, 3, 9] and a fleet of 23 vehicles (model years 1994-2001) [6] have shown that K is often negative. A negative value of K implies that OI exceeds RON for fuels of greater sensitivity, indicating a lower MON value yields greater knock resistance and hence engine performance [10]. Past studies on direct injection spark-ignition (DISI) vehicles [3] have indicated that K decreases for more knock-prone engine conditions, increases with engine speed, and decreases with end-gas temperature for a given pressure. Furthermore, a recent study in a 2007 turbo-charged, direct injection vehicle showed a dependence of the K-value on boosting conditions despite part-load conditions indicating a positive K-value: at full load, wide open throttle (WOT) test conditions, the K-value was found to be negative. As knock is more prevalent at WOT these results are consistent with improved vehicle performance with fuels of high sensitivity [11].

Ultraboost

The Ultraboost project was a collaborative research program involving five industry partners and three universities as specified in Table A.1, co-funded by the UK's innovation agency, the Technology Strategy Board. The aim of the programme was to develop a downsized, boosted engine technology capable of offering a 35% reduction in fuel consumption relative to a production V8 engine, the AJ133 [12], over the New European Drive Cycle (NEDC) in a 2010MY Range Rover vehicle, while maintaining performance and transient response.

Engine design and control system are presented in detail in references [13, 14, 15] and therefore only briefly described here. To achieve a 35% reduction in CO_2 emissions yet maintain the performance of the baseline AJ133 engine (5.0L, naturally aspirated, V8), an inline-4, 2.0L (60% downsized) engine was constructed from one bank of the base engine. A new cylinder head and combustion system were designed, with variable valve timing, cam profile switching, high flow and tumble inlet ports, and both direct injection (DI) and port fuel injection (PFI) capabilities. Cooled external exhaust gas recirculation (EGR) and a water cooled exhaust manifold (WCEM) were also incorporated. Much research has gone into the boosting system, which was designed to be a two-stage series super and turbocharger configuration with an inter- and after-cooler. However, early combustion system optimisation was performed with a charge air handling unit (CAHU) at the University of Bath to simulate the effects of integrated super and turbochargers. To meet the performance target, the first phase of engine development performed with the CAHU was required to meet a 35 and 28 bar BMEP target at 3000 and 2000 rpm, respectively, requiring air charging up to 3.5 bar absolute.

As the Ultraboost concept engine is at the leading edge of downsized, boosted engine technologies, it is useful to understand fuel effects and their impact on performance. In particular, as Ultraboost is expected to have reduced in-cylinder temperature and increased pressure compared to current engines, understanding the octane appetite of this engine provides the opportunity to evaluate the relevance of RON and MON specifications in emerging engine technologies.

In this paper, a series of fuels experiments are described in which air is delivered to the Ultraboost concept engine using a CAHU to simulate the boosting process. An overview of the results on engine response to RON and final engine performance results have been presented in references [16, 17]; this paper follows [16] to describe experimental and theoretical evaluation of the engine's K-value at key regions of engine performance.

EXPERIMENTAL PROCEDURE

Engine Details

The details of the Ultraboost engine and University of Bath test cell are given in Table 2 and the engine installed on the CAHU is shown in Figure 1.

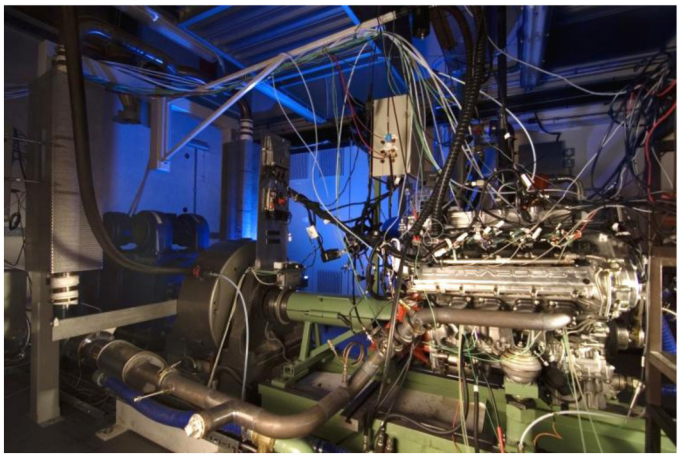


Figure 1. Ultraboost Engine on the dynamometer at the University of Bath

In [17], the engine was shown to provide a 15% improvement in fully-warmed-up fuel economy over the baseline AJ133 V8 which; when friction and engine warm-up were taken into account, together with other secondary vehicle changes, this translated into a >35% reduction in vehicle tailpipe CO_2 on the NEDC. This was achieved using the standard 95 RON pump gasoline which Shell provided throughout the programme for the base engine development programme. Full details of the project and the technologies employed on the Ultraboost engine are provided in [17].

Table 2. Ultraboost Engine and Test Facility Details [18]

Engine Details	
Engine Type	4 cylinder in-line, 4 valves per cylinder
Capacity (cc)	1991
Bore (mm)	83
Stroke (mm)	92
Compression Ratio	9.0:1
Firing Order	1-3-4-2
Construction	All-aluminum AJ133 cylinder block (right bank)
Combustion System	Pent-roof combustion chamber Asymmetrical central DI and spark plug High-tumble intake ports Auxillary port-fuel injection (not used in these experiments)
Valve Train	Chain-driven double overhead camshafts, fast acting dual continuously variable camshaft phasers (DCVCP) Cam profile switching (CPS) tappets on inlet and exhaust
Specific Power	142 (kW/l) @ 6500 rpm
Specific Torque	255 (Nm/l) @ 3500 rpm
Maximum BMEP	~35 bar @ 3500 rpm and ~25 bar @ 1000, 6500 rpm
Other	External cooled EGR, Water cooled exhaust manifold 130-145 bar in-cylinder peak pressure limit
Engine Test Facilities	
Dynamometer	Twin dynamometer arrangement (AVL 215kW AC dynamometer and Froude AG250 Eddy current dynamometer)
Emissions Bench	MEXA 7000 Series with EGR
Cylinder Pressure Sensors	Kistler type 6054 (air cooled)
Cylinder Pressure Acquisition	AVL Indiset

Fuel Properties

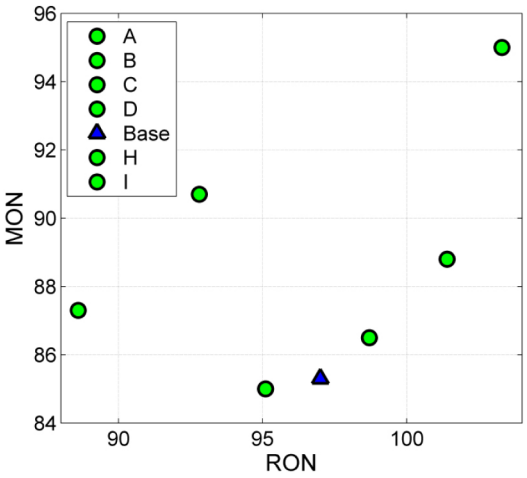
This experiment involved a matrix of 14 fuels designed to screen the Ultraboost engine for performance response to various fuel properties. A subset of 7 of these fuels (Table 3) were formulated to investigate the octane appetite of Ultraboost via decorrelated RON and MON properties (R<0.43), as shown in Figure 2. Though the influence of RON and MON were considered to be the dominant factors in determining engine performance at the knock limit, it should be noted that these fuels also differ by other properties. Base and H are EN228 compliant E5 gasoline fuels; I is an EN228 compliant E0 gasoline. A-D were specifically formulated for maximum RON and MON differences, and are generally not EN228 compliant: A, C and D have low E70[1] and Reid Vapour Pressure (RVP) values; C and D have low densities, and B has slightly high aromatic content. Furthermore, A and B contain methyl-*tert*-butyl ether (MTBE). To further understand fuel differences, the distillation properties of the seven K-value fuels

1. Evaporated volume at 70 °C

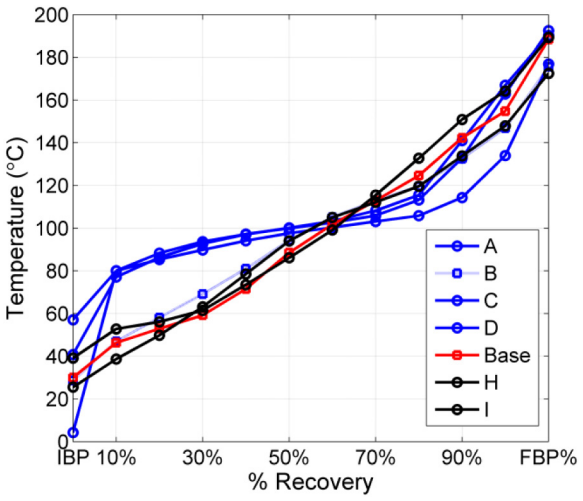
are shown in Figure 2. While Base, B, H and I show similar distillation behaviour, A, C and D are less volatile at low temperatures.

Table 3. Select Properties of Fuel Test Matrix

Fuel	Base	A	B	C	D	H	I
RON	97	103.3	101.4	92.8	88.6	95.1	98.7
MON	85.3	95	88.8	90.7	87.3	85	86.5
S	11.7	8.3	12.6	2.1	1.3	10.1	12.2
Oxygenate Content	E5	14% MTBE	10.5% MTBE	E0	E0	E5	E0
LHV (MJ/kg, gas)	43.1	42.6	42.2	44.3	44.2	43.0	43.3
Density (g/cm^3)	0.743	0.732	0.754	0.703	0.704	0.748	0.735



a. Decorrelated Matrix of RON and MON Fuels. (Correlation coefficient 0.43).



b. Distillation Properties of K-Value Matrix Fuels

Figure 2. Fuel Properties. (a) RON and MON correlation and (b) Distillation properties

Experimental Design

Engine Test Cycle

Four target torque-speed conditions of the engine map were chosen for the fuels experiments, as shown in Figure 3. These conditions were chosen to reflect (1) the supercharged region of engine operation at low speed, high load, (2) the transition between non-boosted and boosted at low speed, mid load, (3) the transition between the super and turbo-charged region of engine operation at mid-speed, high load[2], and (4) the turbo-charged region of engine operation at high speed, high load.

For each of the four torque-speed conditions, one parameter was varied to probe:

1. The effect of external EGR at (1), via test 1A (low) and 1B (high).
2. The influence of boost temperature at (2), via 2A (low) and 2B (high).
3. Back pressure effects at (3) via test 3A (low) and 3B (high).
4. Effect of lambda at (4), via test 4A (stoichiometric) and 4B (rich).

Though the full experimental procedure is described here, the results of test region (1) and (3) only are the focus of the current paper, as these knocking regions of the engine map were used to determine the engine K-values. The detailed engine test conditions are given in Table 4. The target torque was set to be slightly lower than the torque curve target at this engine speed due to in-cylinder pressure limitations. The boost pressures used for the 0% and 10% EGR conditions at test point (1) were set such that similar torques could be achieved at both EGR rates. The boost pressures were initially set with the engine running on base fuel and the chosen boost pressures were subsequently imposed for all remaining fuel formulations

Each fuel was run through the test cycle in a fixed order: 1A, 1B, 2A, 2B, 3A, 3B, 4A and 4B. At test conditions (1) and (3), spark timing (ST) was varied until knock limited spark advance (KLSA) was approximately reached. KLSA was determined by the average knock peak (KP) of the four cylinders as computed via the standard AVL algorithm for knock identification[3]; 10 data points from the initial ST to the KLSA were collected. Within each test condition and ST value the engine was stabilised for 30 seconds before measurement. In-cylinder data (ST, KP, mean effective pressure, maximum in-cylinder pressure, and combustion phasing) was collected and averaged over 10 seconds

2. Due to material limitations of in-cylinder pressure limits at the 3000 rpm condition, the engine operation condition was adjusted to allow for knock limited, rather than in-cylinder pressure limited, experiments: the air charge temperature was increased from 40°C to 60°C to increase the propensity to knock. The inlet cam phasing was also reduced to retard from 60° to 45° reducing the valve overlap and air flow so that KLSA was reached before maximum pressure limit. The maximum BMEP at this operating condition is 32 bar BMEP; the BMEP at this test condition ranged from 19 to 27 bar across the spark sweep.
3. Knock peak is defined as the maximum knock amplitude of the 5kHz - 25kHz band-pass filtered in-cylinder pressure trace.

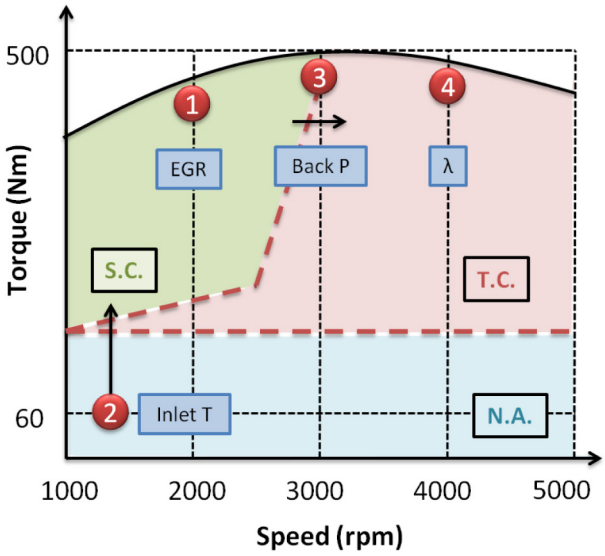


Figure 3. Engine Test Cycle. (1) Super-charge bias with variable EGR; (2) Non-boosted with variable inlet air temperature, (3) Transition between super- and turbo-charger bias with variable back pressure, and (4) Turbo-charger bias with variable λ. (1) and (3) are the focus of the current study.

Table 4. Details of Engine Test Cycle

Condition	1A	1B	3A	3B
Speed	2000		3000	
BMEP (bar) [ST Dependent]	25-31		21-26	
Boost Pressure (bar)	2.3	2.5	2.4	
Back Pressure (bar)	1.45		1.7	2.2
EGR %	0	10	10	
Boost Temperature (˚C)	40		60	
λ	1.0		1.0	
Within test variable	ST to KLSA		ST to KLSA	
Data points	10		10	

Fuels Test Matrix

Each fuel test was repeated once, with the exception of the base fuel, which was tested five times over the course of the experiment to establish an understanding of repeatability and engine drift, and Fuel A, which was tested twice during the course of the experiment.

At four points in the test matrix, the engine was flushed with fresh 5W-20 grade lubricant followed by a fixed 9-hour degreening procedure (4 repeats of the test cycle defined in Table 4). The fuels were tested in order of alternating high and low RON; approximately 1.5L of fuel was used to flush the system and stabilisation of engine response was monitored at a set condition (mid-load, 2000 rpm). The fuels matrix test order is shown in Table 5.

Table 5. Fuels Matrix Test Order. A subset of fuels results are presented in this paper.

Test	Fuel	Test	Fuel
Lubricant Degreening		10	**Base**
1	**Base**	11	A
2		12	
3	H	13	
4	I	Lubricant Degreening	
Lubricant Degreening		14	**Base**
5	**Base**	15	
6	A	16	
7	C	17	
8	B	18	
9	D	19	**Base**
Lubricant Degreening			

K-Value

Experimental

The engine K-value has been determined for a range of engine technologies in previous studies; details regarding these experiments are given in references [1, 3, 4, 6, 7, 11]. In general, this method relies on measuring a performance variable relating to a fuel's auto-ignition propensity for a range of RON and MON decorrelated fuels. In this study, the KLSA[4] was used to determine the K-value from the 7 fuels shown in Figure 2.

K was determined as follows: A linear relationship between KLSA and OI was assumed, such that: $KLSA = \alpha + \beta \times OI_0$. Equations (2), 3, (4) were used to determine this multivariable linear regression.

$$KLSA = a \times RON + b \times MON + c \quad (2)$$

$$K_0 = \frac{b}{a+b} \quad (3)$$

$$OI_0 = RON - K_0 \times S \quad (4)$$

However, as consistent with the results of previous studies [19], the data indicated a quadratic relationship would define a better fit between KLSA and OI, such that:

$$KLSA = \alpha + \beta \times OI + \gamma \times OI^2 \quad (5)$$

K was determined iteratively; an initial guess based upon the linear assumption was used to generate an initial OI; K was then modified to minimize the sum of squared residuals between the experimental and predicted KLSA in equation (5).

4. The knock limited torque, CA50, acceleration time, vehicle tractive effort, fuel efficiency, or the 10% heat release rate have also been used to derive octane appetite.

Theoretical

A method for predicting the K-value of an engine condition from an experimental pressure trace is described in detail in reference [5] and therefore only given briefly here.

An experimental knocking pressure trace was selected for a given engine condition and assumed to be independent of simulation fuel composition. The mass fraction of in-cylinder residuals was estimated via the Shayler method [20].

The in-cylinder temperature of the end-gas was computed using three different methods:

1. As consistent with previous studies [5], the temperature pre-spark was calculated using the mass-based ideal gas law, and the temperature post-spark was calculated using isentropic compression in COSILAB [21]. The in-cylinder temperature of the end-gas was also assumed to be fuel-independent, and taken as the average temperature of that computed for 100% toluene and 100% iso-octane.
2. The temperature was calculated by assuming that, at −360 CA°, in-cylinder gas temperatures are equivalent to experimental inlet manifold temperatures. Adiabatic expansion and compression calculations were then performed using *COSILAB* software, assuming an air plus residual composition until start of injection (SOI), and an air-fuel mixture after SOI.[5]
3. The temperature was modelled with *GT Power* using the in-cylinder pressure trace, airflow and a surrogate fuel[6] composition as input to predict an estimated burn rate and model pressure trace. The model parameters were then iteratively adjusted to minimize the difference between experimental and predicted pressure trace and then used to calculate the in-cylinder unburned gas zone temperature.

Once the temperature was calculated using one of the above simulation methods, for each temperature and pressure condition experienced by the end-gas, COSILAB was used in combination with a toluene, n-heptane, ethanol and iso-octane semi-detailed chemical kinetics mechanism [22] to predict the auto-ignition delay time, τ, for constant volume combustion of a given theoretical fuel formulation and in-cylinder residual content (as estimated by the Shayler method [20].)

The Livengood-Wu assumption:

$$\int_{t=0}^{t_{auto}} \frac{1}{\tau} dt = 1 \qquad (6)$$

was then used to predict the crank angle of auto-ignition (CA_{auto}) for that fuel. This procedure was performed for a series of primary reference fuels (PRF), for which OI=RON=MON, to derive a calibration curve between OI and CA_{auto}. Subsequently, a series of toluene / n-heptane mixtures with predicted RON and MON values were used to compute CA_{auto}, derive OI from the calibration curve, and compute K via equation (7).

$$K = \frac{RON - OI}{RON - MON} \qquad (7)$$

RESULTS AND DISCUSSION

Engine Boundary Conditions

The values for boost temperature, boost pressure, back pressure and EGR were evaluated by averaging over all the data collection points in order to assess stability of test results and understand potential causes for drift. In general, engine conditions were found to be stable and in alignment with the test conditions specified in Table 4, with the exception of increasing engine blow-by over the course of the fuels testing matrix, potentially related to engine aging.

Furthermore, it should be noted that Fuel A was repeated twice, as, during the course of the experiment, lower than target back pressure was shown for the engine condition in test region 3B. However, no data was discarded in this study; the data for both repeats of fuel A were pooled for calculation of key properties. As lower than target back pressure also occurred for fuel D in test region 3B, comparisons of this engine condition with that of 3A should be interpreted with caution.

Knock Limited Spark Advance

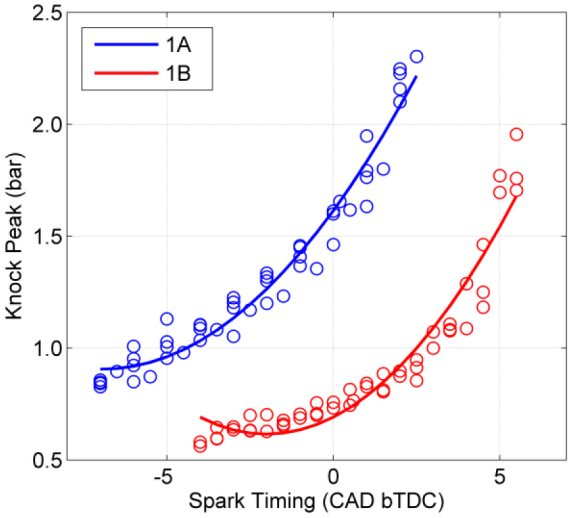
In general, the KLSA was determined as follows. The AVL knock peak as a function of spark timing was averaged over the four cylinders. A quadratic function was used to fit KP against ST, and used to define the ST at which KP was equal to 2 bar (at 2000 rpm, 1A and 1B) or 3 bar (at 3000 rpm, 3A and 3B). For fuels with more than one test repeat, the data of the multiple runs was pooled and a quadratic function fit to the pooled data. This was performed for the base fuel (5 repeats) and fuel A (2 repeats); in both cases, the KP versus ST relationship was very repeatable over the multiple fuels tests. The relationship between KP and ST for the pooled base fuel data is shown in Figure 4; the KLSA results for all 7 fuels are given in Table 6.

The addition of 10% cooled external EGR at the 2000 rpm condition (1B compared to 1A) resulted in a lower knock peak at a given spark timing and hence an advanced KLSA (Figure 4). At 3000 rpm, there was little difference in the KP-ST relationship for the base fuel; at 2.2 bar back pressure (3b) there appeared to be a slightly reduced knock peak and hence advanced KLSA in comparison to the 1.7 bar reference condition (3A).

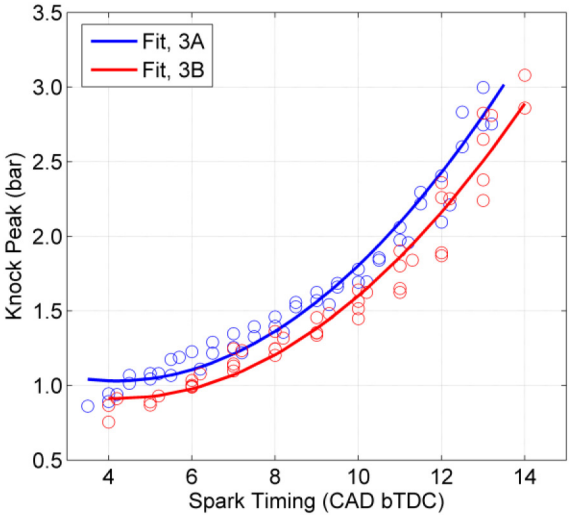
5. The final temperature profile after SOI was derived from the average of the temperatures evaluated for 100% toluene and 100% iso-octane.
6. The surrogate fuel composition was a 95.1% Indolene/4.9% Ethanol mixture which closely matches the physical properties of the base fuel.

Table 6. Knock Limited Spark Advance for Test Fuels.

Fuel	1A	1B	3A	3B
A (Pooled)	3.75	8.23	19.38	19.83
B	4.47	11.46	18.42	18.61
C	-1.50	3.83	9.62	9.86
D	-1.00	3.88	8.89	9.32
Base (Pooled)	1.69	6.56	13.46	14.27
H	1.26	5.77	12.85	12.74
I	3.22	7.71	14.50	14.87



(a). Region 1A and 1B: 2000 rpm



(b). Region 3A and 3B: 3000 rpm

Figure 4. Base Fuel Knock Limited Spark Advance

Octane Appetite

Experimental Results

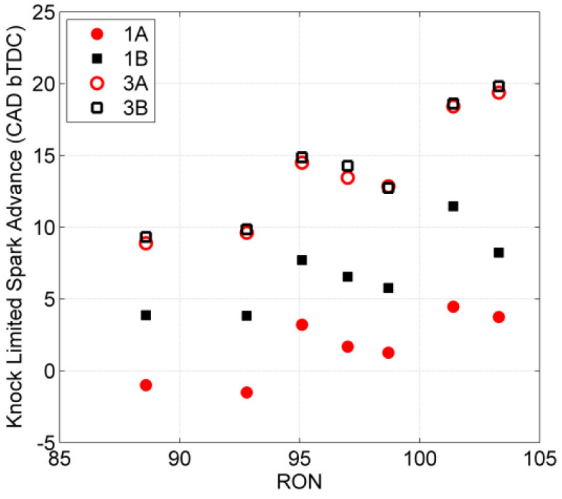
The K-value for each engine condition, and octane index for each fuel at each engine condition, was determined from the KLSA results as discussed above. While KLSA shows some dependence on RON, there is little correlation between KLSA and MON at any of the engine conditions. However, OI and KLSA show a clear quadratic relationship at all engine conditions, as shown in Figure 5[7].

The K-value results for each engine condition are given in Table 7. In general, K is negative, indicating that for a given RON, a fuel of higher sensitivity (lower MON) would exhibit more knock resistance, and hence, allow for improved engine performance.

At 2000 rpm, (1), the K-value was evaluated to be −0.85 and −1.14 for 0 and 10% EGR, respectively. The 10% EGR condition was calculated to have a more negative K-value, indicating a larger benefit for fuels of higher sensitivity relative to the 0% EGR case. The more negative K-value with increased EGR could be due to a combination of reduced in-cylinder temperature and the higher boost pressure at this condition.

At 3000 rpm, (3), the K-value was evaluated to be −0.20 and −0.21 for low and high back pressure, respectively, potentially indicating little to no difference in octane appetite as a result of transitioning from the super- to turbo-charger bias region of the engine map. However, due to the low back pressure conditions for fuels A and D at 3B, definitive conclusions from this test condition cannot be made.

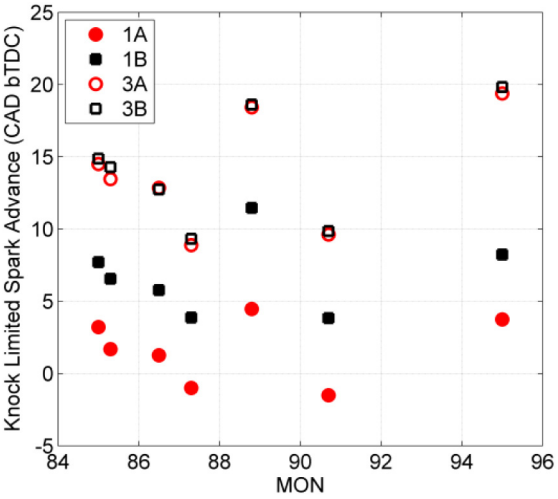
The K-value was found to be more negative at region (1) in comparison to region (3), indicating that at lower engine speeds more prone to knock, fuels of greater sensitivity would provide a larger benefit.



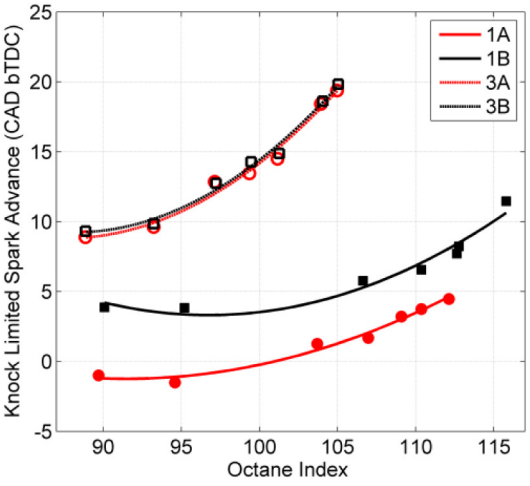
(a)

Figure 5. Dependence of KLSA on (a) RON, (b) MON and (c) Octane Index.

7. Note that the slope of the quadratic when fitting an engine-out performance variable (e.g. acceleration time, brake specific fuel consumption, power, etc) is generally expected to be opposite to the trend observed here; i.e. a decrease in performance with increase in OI as the performance limit of the engine is achieved or minimum advance for best timing (MBT) is reached. However, no such limit exists for KLSA and it is theoretically possible to continue advancing the spark timing with fuels of increasing resistance to auto-ignition; therefore the positive quadratic shown in Figure 6 is a physically meaningful result. However, the minimum observed for Region 1B at mid-octane levels is not expected to be physical, but an artefact of the quadratic fitting procedure.



(b)



(c)

Figure 5. (cont.) Dependence of KLSA on (a) RON, (b) MON and (c) Octane Index.

Table 7. Octane Appetite, K, at Regions (1) and (3)

Region	Engine Condition	K-value
1A	0% EGR, 2.3 bar boost	-0.85
1B	10% EGR, 2.5 bar boost	-1.14
3A	1.7 bar back pressure	-0.20
3B	2.2 bar back pressure	-0.21

For a more rigorous comparison of the K-values at the different engine operating conditions, the 95% confidence intervals were assessed (Figure 6). The fuels matrix used for octane appetite evaluation was relatively limited, leaving few experimental degrees of freedom and hence large uncertainty, rendering rigorous comparisons between different engine conditions difficult. The K-value at test condition (1A) was found to be negative at the 95% confidence level (CL). However, no statistically significant difference was observed between the four test conditions at the 95% CL.

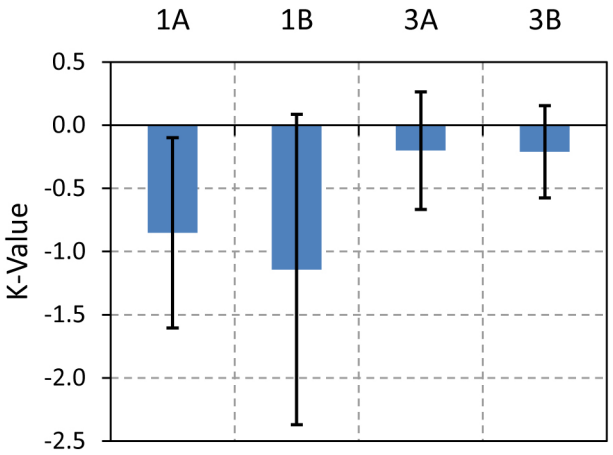


Figure 6. 95% Confidence Intervals of K-values

These results are in broad agreement with previous studies, where the octane appetite of modern, direct injection engines has been shown to be generally negative or close to zero at similar engine conditions. In a 23 vehicle study, Kalghatgi [6] determined the K-value for a range of vehicles including those fitted with direct injection technology. These vehicles exhibited K-values ranging from −0.52 to 0.05. In an additional study using a 2.0L GM Ecotec direct injection engine, a K-value of −0.75 was determined at full load conditions [11]. The Ultraboost engine results are thus in agreement with these experiments; the K-values for highly downsized, boosted direct injection engines such as Ultraboost are expected to decrease as the in-cylinder pressure increases and temperature decreases relative to traditional port-fuel injection, naturally aspirated technology.

Further studies have been performed with a GM Ecotec engine fitted with turbo-charging and EGR systems. Results from this study by Davies *et al.*[9] show that a K-value of −0.86 was obtained at 2000 rpm and 0% EGR fraction. With 10% EGR at identical conditions, the K-value was found to increase to −0.39.

By contrast, in this study the K-value decreases with the addition of EGR, in apparent contradiction to previous results [9]. This may be due to the higher boost pressure at this condition required to obtain the fixed torque target at the 10% EGR condition. Indeed, upon inspection of the pressure and predicted temperature profiles for 1A and 1B, the 0 and 10% external EGR conditions, the latter exhibits a higher pressure and a lower temperature than the former, and it is therefore consistent with the expectation that at a given engine condition, a decrease in the in-cylinder temperature will result in a decrease in the K-value [8][5].

8. In this experiment, each test condition was principally defined using boost pressure and engine speed targets. In the previous work by [19], each test condition was defined using brake torque and engine speed targets; therefore boost pressure was allowed to be varied between fuels at the same test condition. This difference in approach may have an impact on derived K-value. Note that at the 10% EGR condition, a higher, fixed boost pressure was used throughout to enable an iso-torque comparison to the 0% EGR condition.

Theoretical Results

In addition to the K-values derived from experimental KLSA data, K-values were simulated at conditions 1A and 1B by employing the method of Davies *et al* [5] and selecting the most knocking pressures traces from the first base fuel repeat (Figure 7).

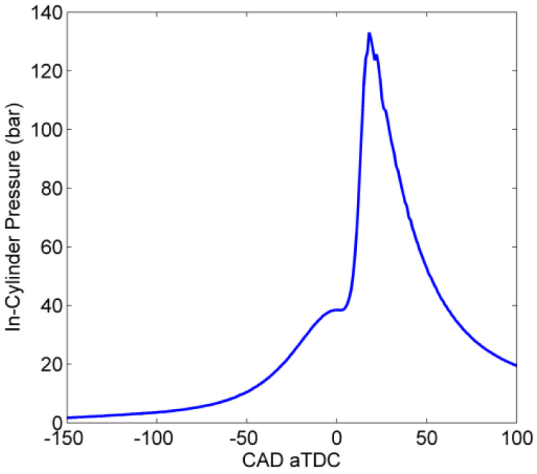


Figure 7. Knocking pressure trace selected from engine test condition 1A, first repeat of base fuel.

The K-value method relies on an accurate prediction of the in-cylinder temperature of the unburned end-gas at each volume-pressure condition to predict the auto-ignition delay time and hence the crank angle of auto-ignition. The assumptions and methods used to calculate the in-cylinder temperature of the unburned gas have a large impact on the final temperature profile (Figure 8).

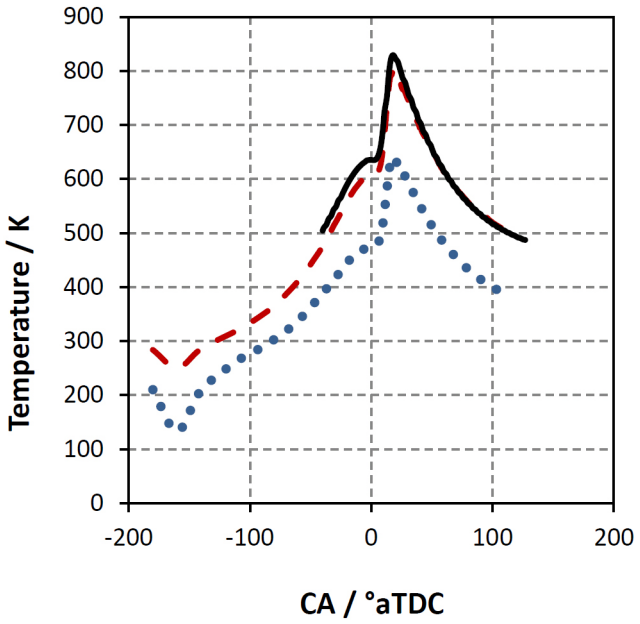


Figure 8. Derived temperature profiles from the 1A experimental pressure trace. (1) Blue, dotted: Ideal gas law and adiabatic compression from spark, (2) Red, dashed: Adiabatic expansion / compression from inlet manifold starting temperature, and (3) Black, solid: GT-Power modelled temperature.

The temperature simulation method (1), based on ideal gas and adiabatic compression from the spark, resulted in an extremely low temperature profile (Figure 8, blue dotted line). Temperatures of 133K are unrealistically low and at these temperature conditions, the Livengood-Wu integral method predicted that even very low-octane PRF fuels would not knock. Therefore this approach was deemed unsuitable for application to the Ultraboost engine data.

The temperature profiles derived from the adiabatic expansion/ compression method (2) and the GT power methodology (3) are higher and hence more realistic. Small differences are observed between the two profiles with the GT power model predicting slighter higher temperatures (Figure 8). The GT-Power model temperature method was selected to calculate the final K-values due to increased accuracy of the model in predicting the effect of 10% EGR on in-cylinder temperatures in test region 1B.

Following derivation of the in-cylinder temperature profile, a calibration curve was generated by determining the crank angle of knock onset for PRF fuels. The calibration curve (fuel OI versus CA_{auto}) generated for condition 1A using the GT power temperature profile (3) is given in Figure 9.

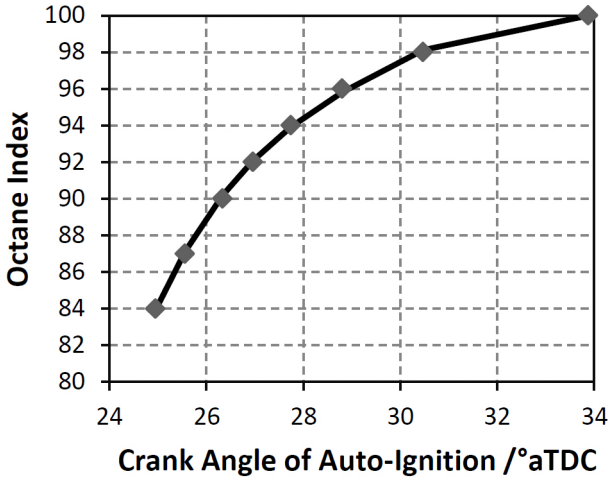


Figure 9. Calibration curve (polynomial fit) to Livengood-Wu integral predicted auto-ignition crank angle for PRF fuels for Region 1A using GT Power temperature simulation method (3).

The shape and range of the calibration curve as shown in Figure 9 is a function of the engine design and the specific temperature-pressure history of the end-gas. The calibration curve is used to predict the K-value by determining the crank-angle of auto-ignition via the Livengood-Wu method for a toluene/heptane fuel mixture of known RON and MON, predicting the OI using the calibration curve, and back-calculating the K-value. The K-value is an engine dependent parameter and hence should depend solely on engine condition and not fuel. However, due to the steep gradient of the calibration curve at low values of fuel OI, inaccuracies in K-value prediction can occur such that an increase in K-value is predicted with a decrease in the OI of the fuel used to compute K. In this experiment it was therefore

decided to assume the region of the calibration curve between 92 < OI < 98 to be linear and only use this portion of the curve to predict K.

Using the temperature profiles obtained from GT-Power, the K-value results for conditions 1A are given in Table 8. The average results for test conditions 1A and 1B are given in Table 9.

Table 8. Octane Appetite, K, at condition 1A, for a series of Toluene / Heptane blends with OI between 92 to 98.

Toluene / vol%	Heptane / vol%	RON	MON	t_auto / (CAD)	OI	K
74	26	92.9	78.7	22.3	97.2	-0.31
72	28	90.8	76.8	21.5	93.7	-0.21
Average						-0.26

Table 9. Average Octane Appetites, K, at conditions 1A and 1B, for a series of Toluene /Heptane blends.

Condition	% EGR	Predicted K-value	Experimental K-value
1A	0	-0.26	-0.85
1B	10	-0.35	-1.14

The simulated K-values agree with the experimental K-values, in that they are both negative and that the K-value decreases with external EGR. However, while the trends agree, the theoretical predictions are smaller in magnitude than experiment. This discrepancy may be due to differences in the experimental and theoretical methodologies. One possible cause of this difference is that theoretical K-values are derived from the analysis of a single pressure trace from one cylinder, while the experimental KLSA is determined by applying a band pass filter and averaging the subsequent knock peak over the four cylinders. Therefore if the selected pressure trace is dissimilar to the knock peak average, differences between the experimental and theoretical values may arise.

In a previous application of the K-value simulation methodology to the EGR-Boost engine (2.0L 4-cylinder Direct Injection with external EGR [9]), good agreement between the experimental and theoretical K-values were obtained, and both theory and experiment indicated an increase in K with external EGR, in contrast to observations from this study. However, a number of experimental factors make direct comparison between these studies difficult. In the Ultraboost experiment, while the boost pressure between 0% and 10% EGR conditions was adjusted to achieve the same target torque, boost pressure was held constant between different fuels to determine KLSA due to the torque control capabilities of the engine control unit and test cell. In contrast, the EGR-Boost program was target-torque controlled for all fuels.

The K-value simulation method has been extended in this study and used to reproduce trends regarding the determined K-values for a downsized, highly-boosted prototype engine, confirming both that these engines tend towards negative K-values and that this is a result of increased in-cylinder pressure and decreased temperature. To further refine the model and increase its predictive power for future application, improvements can be made to the input parameters and pressure-trace selection. This study found that in-cylinder temperature prediction is best obtained from a calibrated engine model. Furthermore, additional improvements could be made in selecting pressure traces, such as applying a band filtering and averaging function to experimental results to obtain a pressure trace representative of global engine performance, or selecting pressure traces based on different criteria; e.g. the pressure trace with the fastest combustion.

Sensitivity and Performance

The negative K-value for the Ultraboost engine implies that for a fixed RON, a fuel with a lower MON and therefore higher sensitivity will yield a larger OI, and hence better knock resistance. In an engine with an octane responsive engine management system (EMS), the fuel with the higher OI will in turn yield better engine performance.

Fuels A and B were selected for additional analysis to probe the influence of sensitivity on fuel performance for the different K-value regimes. The OI for each of the fuels was computed from the experimental K-values; performance variables at the knock limit were computed by fitting quadratic functions to the data against spark timing, as for KP.

At the knock limited 2000 rpm condition, for both 0 and 10% EGR, fuel B was found to have a higher octane index than fuel A, despite the fact that fuel A has higher RON and MON values. This is due to the higher sensitivity of fuel B, which makes this fuel less prone to knock at this condition, allowing for a more advanced spark timing and hence BMEP benefit (Table 10).

At the less knock limited, 3000 rpm condition, fuel A was found to have a higher OI than fuel B; for the lower K-value of approximately −0.2, a sensitivity difference of 4.3 was not found to offset the RON difference of 1.9. Hence fuel A was found to have a slightly higher OI and therefore also a more advanced KLSA. Despite the more advanced KLSA at region (3), fuel B was found to still yield a BMEP benefit; this was largely attributed to a decreased 50-10 combustion duration due to a lower level of MTBE in the fuel formulation; this effect was more noticeable at 3000 rpm than the 2000 rpm condition. However, despite this deviation, in both cases, the higher OI corresponded to a more advanced KLSA.

Table 10. Comparison of fuels A and B at KLSA

Property	Fuel A	Fuel B	Difference (B-A)	
RON	103.3	101.4	-1.9	
MON	95	88.8	-6.2	
Sensitivity	8.3	12.6	4.3	
Fuel A				
	1A	1B	3A	3B
OI	110.36	112.76	104.96	105.04
KLSA (CAD)	3.75	8.23	19.38	19.83
BMEP (bar)	29.70	30.28	25.81	24.63
Fuel B				
OI	112.11	115.76	103.92	104.05
KLSA (CAD)	4.47	11.46	18.42	18.61
BMEP (bar)	29.95	30.66	26.06	24.81
Comparison				
OI	1.76	3.00	-1.04	-1.00
KLSA (CAD)	0.72	3.23	-0.96	-1.22
BMEP (bar)	0.83%	1.24%	0.94%	0.74%

CONCLUSIONS

Modern engine technologies are diverging from the traditional CFR engine on which the RON and MON octane rating scales are based, specifically with respect to in-cylinder temperature and pressure conditions which have a direct impact on a fuel's auto-ignition propensity. The octane index, which relies on an engine and condition-dependent factor, K, is a superior measure of predicted auto-ignition resistance of a fuel in a given engine, and hence of the anticipated performance benefit of that fuel.

The Ultraboost engine is a highly boosted, downsized, 4-cylinder prototype engine designed to realize a 35% benefit in CO_2 emissions whilst maintaining performance of a baseline naturally aspirated V8. The K-value was determined at 4 different engine conditions using the knock-limited spark advance from a matrix of RON and MON decorrelated fuels. The K-value was found to be negative at all engine conditions. Furthermore, the K-values were simulated using an experimental pressure trace and an improved temperature prediction method. The simulated K-values correlate with the trends observed in the experimental data for regions 1A and 1B.

A case study of fuels of varying sensitivity showed that a fuel's auto-ignition resistance was indeed reflected by using OI as a key parameter; in general, at the knock limited high load engine conditions probed in this study, fuels of higher sensitivity are important for increased knock resistance, and, in the absence of secondary fuel effects seen in this study such as flame speed, performance.

The evolution of modern engines towards further downsized and boosted configurations, in combination with the results from this study, challenges the relevance of a lower limit to the MON specification for engine performance. This study has shown that the K-value is negative across a variety of engine conditions and that auto-ignition resistance of a fuel is best with high RON and high sensitivity formulations. Under these conditions, engine performance could be limited by the presence of a lower limit for the MON specification.

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ACKNOWLEDGMENTS

The authors gratefully acknowledge the co-funding of the work by the Technology Strategy Board. We also acknowledge the contributions throughout engine development and the testing program of consortium members GE Precision Engineering, Lotus, CD Adapco, University of Leeds, and Imperial College London. Though too numerous to mention by name, we acknowledge our many colleagues at Shell Technology Center Thornton and Shell Technology Center Hamburg in Fuels Blending, Fuels Laboratory, Analytical and Statistics, for making this experiment possible.

DEFINITIONS/ABBREVIATIONS

BMEP - Brake mean effective pressure

CAHU - Charge air handling unit

CFR - Cooperative fuels research

CL - Confidence level

DI - Direct injection

DISI - Direct injection spark ignition

EGR - Exhaust gas recirculation

EMS - Engine management system

K - Octane appetite

KLSA - Knock limited spark advance

KP - Knock peak

MBT - Minimum advance for best torque

MON - Motor octane number

NEDC - New European drive cycle

OI - Octane index

PFI - Port fuel injection

PRF - Primary reference fuel

RON - Research octane number

S - Sensitivity

ST - Spark timing

WCEM - Water cooled exhaust manifold

APPENDIX

Table A.1. Industry and University Partners of the ULTRABOOST Project

Partner	Role in Collaboration
Jaguar Land Rover	(JLR) was the lead partner, with responsibility for engine build, general procurement, engine mounted charging system integration and overall project management.
GE Precision Engineering	Provided engine design and machining capabilities as well as background knowledge on the design of high-specific-output racing engines.
Lotus	Provided dedicated engine management systems (EMS), 1-D modelling and know-how on pressure charged engines, and support for engine testing.
CD Adapco	Supported the design process with steady-state and transient CFD analysis primarily in order to support intake port design.
Shell Global Solutions (UK)	Provided knowledge of auto-ignition phenomenon, base fuel for engine development including full fuel analysis, detailed lubricant analysis to aid in interpretation of engine wear, and designed and interpreted a test matrix of fuel formulations in a thorough program to screen engine response to various fuel properties.
University of Bath	Conducted all of the testing, having dedicated boosting and cooled exhaust gas recirculation (EGR) rigs which were used for the initial testing of the demonstrator engine and for fuels testing work.
University of Leeds	Developed their auto-ignition model to assist with the 1-D modelling process.
Imperial College London	Specified the charging system components, with support from both JLR and Lotus, and tested them in order to characterise them accurately so that the 1-D model was as robust as possible.